CLAIMS :

1. A method for selecting a compound capable of binding to a tyrosine kinase domain of an insulin-like growth factor-l (IGF1) receptor, comprising:

(a) determining an ability of a test compound to fit into a three-dimensional structure formed by the tyrosine kinase domain of the IGF1 receptor; and

(b) selecting a test compound predicted to fit the three-dimensional structure.

2. The method of claim 1, wherein the method is computer-assisted.

3. The method of claim 1, wherein the three-dimensional structure is the tyrosine kinase domain of the IGF1 receptor described by the coordinates of APPENDIX A.

4. The method of claim 1, wherein the IGF1 receptor comprises the sequence of SEQ ID NO: 1.

5. The method of claim 3, wherein the tyrosine kinase domain of the IGF1 receptor comprises amino acid residues 992-1292 of SEQ ID NO: 1.

6. The method of claim 2, wherein the computer-assisted method comprises virtual ligand docking and screening techniques capable of designing and/or identifying a compound predicted to bind a three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor.

7. The method of claim 6, wherein the three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor is selected from the group consisting of an ATP-binding pocket, a peptide substrate binding groove, a hinge region on the backside of the kinase domain, and an alpha helix C.

8. The method of claim 6, wherein the compound predicted to bind to a three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor is predicted to bind with high affinity.

9. The method of claim 6, wherein binding to a three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor is predicted to modulate an activity of the IGF1 receptor.

10. The method of claim 9, wherein modulating an activity of the IGF1 receptor reduces or inhibits an activity of the IGF1 receptor.

11. The method of claim 9, wherein modulating an activity of the IGF1 receptor increases or prolongs an activity of the IGF1 receptor.

12. A method of discriminating between compounds capable of binding to an insulin-like growth factor 1 (IGF1) receptor or an insulin receptor, comprising:

(a) determining an ability of a test compound to fit into a three-dimensional structure formed by a tyrosine kinase domain of the IGF1 receptor;

(b) determining an ability of the test compound to bind the insulin receptor; and

(c) selecting a test compound predicted to fit a three-dimensional structure formed by the tyrosine kinase domain of the IGF1 receptor, said test compound not capable of binding to the insulin receptor.

13. A computer-assisted method for designing a compound capable of binding a tyrosine kinase domain of an insulin-like growth factor-l (IGF1) receptor, comprising:

(a) determining an ability of a test compound to fit into a three-dimensional structure formed by the tyrosine kinase domain of the IGF1 receptor (IGF1RK);

(b) generating the test compound;

(c) contacting the test compound with the three-dimensional IGF1RK structure; and

(d) determining if the test compound binds IGF1RK.

14. The method of claim 13, wherein the three-dimensional structure is the tyrosine kinase domain of the IGF1 receptor described by the coordinates of APPENDIX A.

15. The method of claim 13, wherein the tyrosine kinase domain of the IGF1 receptor comprises amino acid residues 992-1292 of SEQ ID NO: 1

16. The method of claim 13, wherein the computer-assisted method is virtual ligand docking and screening techniques capable of designing and/or identifying a compound predicted to bind to a three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor.

17. The method of claim 16, wherein the three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor is selected from the group consisting of an ATP-binding pocket, a peptide substrate binding groove, a hinge region on the backside of the kinase domain, and an alpha helix C.

18. The method of claim 13, wherein binding of the test compound to the IGF1RK is predicted to modulate an IGF1 receptor activity.

19. The method of claim 18, wherein binding of the test compound to the IGF1RK is predicted to reduce or inhibit an IGF1 receptor activity.

20. The method of claim 18, wherein binding of the test compound to the IGF1RK is predicted to enhance or prolong an IGF1 receptor activity.

21. The method of claim 18, wherein the IGF1 receptor activity is tyrosine kinase activity.

22. A computer-assisted method for designing a molecule capable of modulating an activity of an insulin-like growth factor-l (IGFl) receptor, comprising:

(a) determining an ability of a test molecule to fit into a three-dimensional structure formed by a tyrosine kinase domain of the IGFl receptor;

(b) selecting the test molecule predicted to bind the tyrosine kinase domain of the IGF1 receptor;

(c) generating the test molecule;

(d) contacting the test molecule with the three-dimensional IGF1RK structure; and

(e) determining if the test molecule binds IGF1RK, wherein a test molecule capable of binding to the IGF1RK and modulating an activity of the IGF1RK is a modulator of the IGF1 receptor.

23. The method of claim 22, wherein the three-dimensional structure is the tyrosine kinase domain of the IGF1 receptor having coordinates of APPENDIX A.

24. The method of claim 22, wherein the tyrosine kinase domain of the IGF1 receptor comprises amino acid residues 992-1292 of SEQ ID NO: 1

25. The method of claim 22, wherein the computer-assisted method is virtual ligand docking and screening techniques capable designing and/or identifying a compound predicted to bind to a three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor.

26. The method of claim 25, wherein the three-dimensional motif of the tyrosine kinase domain of the IGF1 receptor is selected from the group consisting of an ATP-binding pocket, a peptide substrate binding groove, a hinge region on the backside of the kinase domain, and an alpha helix C.

27. The method of claim 22, wherein the modulator is capable of reducing or inhibiting IGF1RK activity.

28. The method of claim 22, wherein the modulator is capable of increasing or prolonging IGF1RK activity.

29. The method of claim 22, wherein the test molecule is a non-peptide-based molecule or a peptide-based molecule.

30. The method of claim 1, wherein the test compound is a non-peptide-based molecule or a peptide-based molecule.

31. The method of claim 12, wherein the test compound is a non-peptide-based molecule or a peptide-based molecule.

32. The method of claim 13, wherein the test compound is a non-peptide-based molecule or a peptide-based molecule.